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A HIGHER ORDER EXPONENTIAL FUNCTION FOR FITTING NONLINEAR CURVES

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1. INTRODUCTION

The purpose of this technical memorandum is to present the R/K optical profile function and several graphical comparisons that illustrate the power and versatility of the function to fit nonlinear curves. Here, we did not review or present any of the multitude of mathematical curve fitting methods that are presented in numerous texts and papers. Instead, we focused on the R/K functional form that we found to fit most of the vertical profiles of extinction and backscatter coefficients that were simulated by our theoretically based microphysics model (Rachele and Kilmer, 1992). The R/K function did not evolve without considerable effort. We had tried fitting extinction (σ_e) and backscatter (β) profile curves with other standard and nonstandard functional forms and approaches, but we were not consistently successful. One of these approaches involved calculating $\sigma_e(z+h)$ versus $\sigma_e(z)$ data, where z is height above ground level and h is a constant height increment, as proposed by Duncan et al. (1980). Those $\sigma_e(z+h)$ versus $\sigma_e(z)$ data were transformed (by rotation and/or translation of axes), and fitting functions were investigated for the transformed data. Another approach involved two-piece, double-exponential functions (Heaps, 1982; Rachele and Kilmer, 1991; Kilmer and Rachele, 1992a) such as

$$\sigma_{e} = A \exp [B \exp (Cz)]$$
, (1)

where A, B, and C are constants with appropriate values for the case being approximated. The latter approach was one of the more promising, but was not acceptable for our purposes. This was especially true for simulated backscatter coefficient profiles where the structure was too extensive to allow successful fitting by this approach. Specifically, we were searching for a continuous function that would result in a good fit over a wide range of points, while being constrained to fit the end points precisely. In particular, we wanted a function that required a minimum number of fitting constants, and we did not want to fit the entire curve by cutting it into several subsegments. For these reasons, we did not consider fitting with splines to be a desirable option.

2. THE R/K OPTICAL PROFILE FUNCTION

The R/K optical profile function is a higher order exponential written as

$$y = y_1 \left(\frac{y_2}{y_1}\right)^{M(x)}. \tag{2}$$

where

$$M(x) = \left(\frac{x - x_1}{x_2 - x_1}\right)^{N(x)}.$$
 (3)

In equations (2) and (3), x is the independent variable and y is the dependent variable. The constraint points (end points) are designated as (x_1, y_1) and (x_2, y_2) . N(x), a function of x, is represented in general form as

$$N(x) = \exp\left\{a_0 + \sum_{i=1}^{n} a_i x^i\right\}$$
 (4)

or, for curves that contain oscillations.

$$N(x) = A_0 + 2 \sum_{n=1}^{N_A} A_n \cos \left[\frac{2\pi n(x - x_{F1})}{x_{F2} - x_{F1} + 1} \right] - 2 \sum_{n=1}^{N_B} B_n \sin \left[\frac{2\pi n(x - x_{F1})}{x_{F2} - x_{F1} + 1} \right]$$
 (5)

in the range $x_{F1} \le x \le x_{F2}$. In equations (4) and (5), A_o . A_1 through A_{NA} , B_1 through B_{NB} , x_{F1} , x_{F2} , a_o , and a_1 through a_n are constants. In our work we have found that n=3 is

generally sufficient when using equation (4) to fit extinction coefficient profiles; whereas, when fitting backscatter profiles, as many as 31 (= $1 + N_A + N_B$) constants are used in equation (5).

To implement the functional structure defined by equations (2) through (5), we first solve equations (2) and (3) for N(x) giving

$$N(x) = \frac{\ln\left(\frac{\ln y - \ln y_1}{\ln y_2 - \ln y_1}\right)}{\ln\left(\frac{x - x_1}{x_2 - x_1}\right)}.$$
 (6)

Using some sets of N(x) data calculated according to equation (6), In N(x) versus x data were fitted with polynomials to determine values of the constants in equation (4). Some other sets of N(x) data calculated according to equation (6) were fitted using Fourier analysis, resulting in the fitting expression given by equation (5). For some cases, one must use a combination of polynomial and Fourier terms. The polynomial and Fourier constants were determined by using IMSL (International Mathematical and Statistical Library) routines. All of the points (x, y) selected for fitting must be such that $x_1 < x < x_2$. All points used for polynomial fitting of ln N(x) must have y values such that $y_1 < y < y_2$.

3. EXAMPLES AND RESULTS

Values of (xi. yi) simulated by three different physical/mathematical models were considered in this study. For the first example, values (y,) of extinction and backscatter coefficients simulated with the R/K microphysics model were considered. A plot of each of these simulated profiles is shown as solid lines in figures 1 and 2, where z = x is the height above ground. For simulating data used in figure 1, model input included reference height (2 m above ground level) values of 95 percent, 5 km, and 0 °C for relative humidity, visibility, and ambient air temperature, respectively. Near adiabatic conditions and a maritime air mass were also selected. Model input for simulating data used in figure 2 also specified a maritime air mass, but a maximum liquid water content that would be 75 percent of the near adiabatic value was selected, and reference height values of 99 percent, 2 km, and 30 °C were specified for relative humidity, visibility, and ambient air temperature, respectively. These curves were considered as two segments for each case. The first segment represents the subcloud region for 2 m \leq z \leq 103 m for extinction and 2 m \leq z \leq 36 m for backscatter. The second segment represents the cloud region for 104 m \leq z \leq 463 m and 37 m \leq z \leq 460 m for extinction and backscatter, respectively. The fitting curves produced by equation (2) for extinction and backscatter coefficients are shown as dashed lines in figures 1 and 2. We considered the fits in each case to be very good. Values of R² (the coefficient of determination) were 0.99986 and 0.99855 for the fits shown in figures 1 and 2, respectively. The In N(z) for extinction was fit with a cubic polynomial, figure 3. The fitting curve for backscatter shown in figure 4 was calculated by fitting In N(z) with a cubic polynomial for the first segment and fitting N(z) with a 16-term Fourier series for the second segment. Note that even though the N(z) curves in figures 3, 4, and 6 are discontinuous at the cloud base, the corresponding $\sigma_{\rm e}$ and β curves are continuous as shown in figures 1, 2, and 5. As expected, the $\sigma_{\rm e}$ and β curves pass precisely through the specified values at the reference height (2 m), the cloud base, and the cloud top. Overall, the function fits of σ_e and $oldsymbol{eta}$ are very good. We did find, however, that for some cases a large number of Fourier terms were required to obtain a good fit. As an example, 31 Fourier terms were used for the second segment shown in figures 5 and 6.

For the second example, we used data produced by our thermal conductivity model for loam soil, where k_s (= y) is the thermal conductivity and ϕ_w (= x) is the volume fraction of water. When generating the solid line curve shown in figure 7, we assumed that the volume fraction of solid material (sand, silt, and clay) was 0.5 and the volume fraction of organic matter was 0.10. This curve was fit by equation (2) for $0.2 \le k_s \le 2.1$ and $0 \le \phi_w \le 0.27$. Casual inspection shows that the fit is excellent. The $\ln N(\phi_w)$ for this case was fit by a fourth degree polynomial, figure 8.

The third example makes use of a curve produced by our atmospheric planetary boundary layer model.** The solid line in figure 9 shows the change of wind direction α (= y) as a function of height z (= x), where α varies from 13° to 40° for 2 m \leq z \leq 1000 m. The R/K fit to this curve is shown in figure 9. Again the fit is excellent. The ln N(z) values for this case were fit by a fourth degree polynomial, figure 10.

4. CONCLUSIONS

For the examples considered in this study, we found that the R/K optical profile function fits smooth model simulated curves very well. In a separate study (Kilmer and Rachele, 1992b), we fitted several hundred extinction and backscatter coefficient profiles with the R/K optical profile function and reached the same conclusion. Some cases, however, did require more terms than we would have liked when fitting N(z), $\sigma_{\rm e}$, and β . Some backscatter coefficient curves with many large amplitude oscillations are examples of such cases. Some cases required both polynomial and Fourier terms.

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 (Unpublished)

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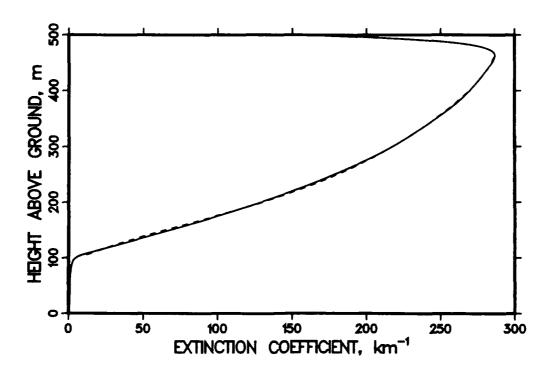


Figure 1. Solid line: R/K microphysics model simulation for a wavelength of 4.0 μ m; dashes: calculated using R/K optical profile function as defined by equations (2), (3), and (4), with x = height, y = extinction coefficient, and n = 3.

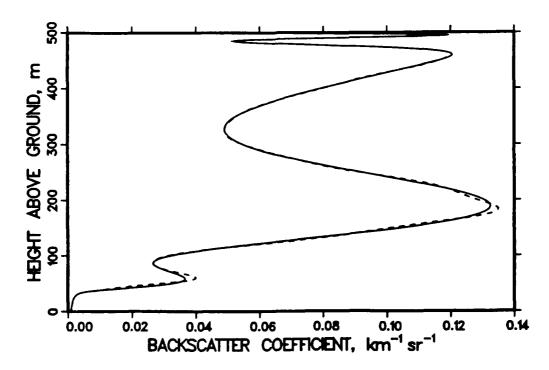


Figure 2. Solid line: R/K microphysics model simulation for a wavelength of 10.6 μ m; dashes: calculated using R/K optical profile function as defined by equations (2), (3), and (4) (for x \leq 36 m) or (5) (for x \geq 37 m), with x = height, y = backscatter coefficient in equation (2), N_A = 8, and N_B = 7.

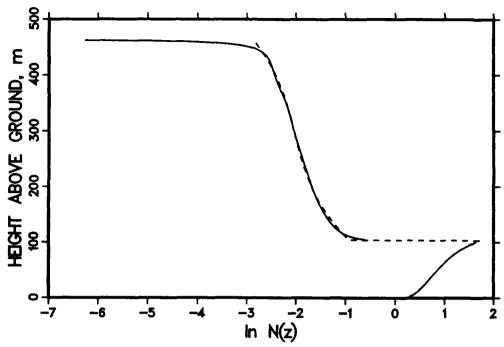


Figure 3. Solid line: R/K microphysics model simulation for a wavelength of 4.0 μ m; dashes: calculated using equation (4), with x = height, y = extinction coefficient in equation (2), and n = 3.

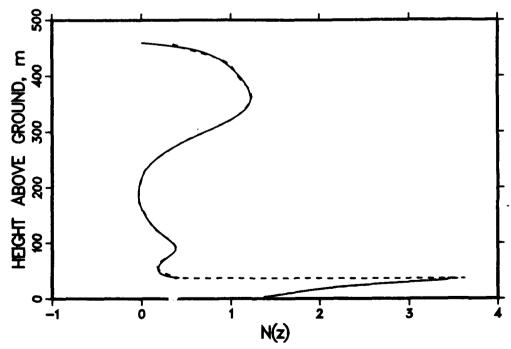


Figure 4. Solid line: R/K microphysics model simulation for a wavelength of 10.6 μ m; dashes: calculated using equation (4) for x \leq 36 m and equation (5) for x \geq 37 m, with x = height, y = backscatter coefficient in equation (2), N_A = 8, and N_B = 7.

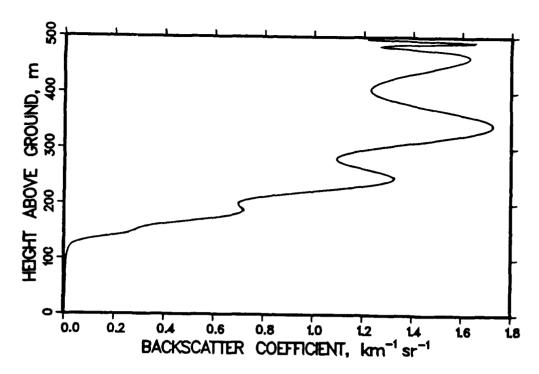


Figure 5. Solid line: "K microphysics model simulation for a wavelength of 5.0 μ m, maritime air mass, near adiabatic conditions, and reference height (2 m) values of 95 percent, 5 km, and 30 °C for relative humidity, visibility, and temperature, respectively. Dashes: calculated using R/K optical profile function as defined by equations (2), (3), and (4) (for x \leq 129 m) or (5) (for x \geq 130 m), with x = height, y = backscatter coefficient, and N_A = N_B = 15.

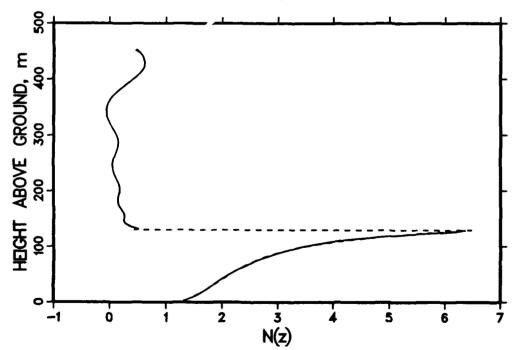


Figure 6. Solid line: R/K microphysics model simulation for same wavelength and case as in figure 5. Dashes: calculated using equation (4) for $x \le 129$ m and equation (5) for $x \ge 130$ m, with x = height, y = backscatter coefficient in equation (2), and $N_A = N_B = 15$.

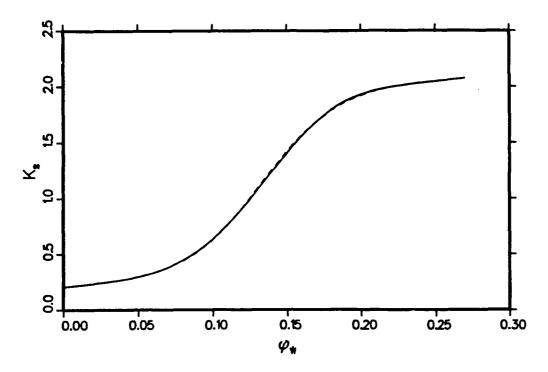


Figure 7. Thermal conductivity vs. water content for foam where $\phi_{\rm s}=0.5,~\phi_{\rm q}=0.2$ \\\ fit with RK optical profile fit N($\phi_{\rm w}$) = exp (0.040407 + 3.3972 $\phi_{\rm w}$ - 17.454 $\phi_{\rm w}^2$ - 769.18 $\phi_{\rm w}^3$ + 2460.47 $\phi_{\rm w}^4$.

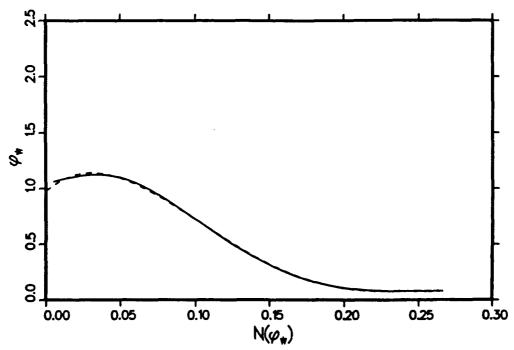


Figure 8. N(z) profile corresponding to figure 7.

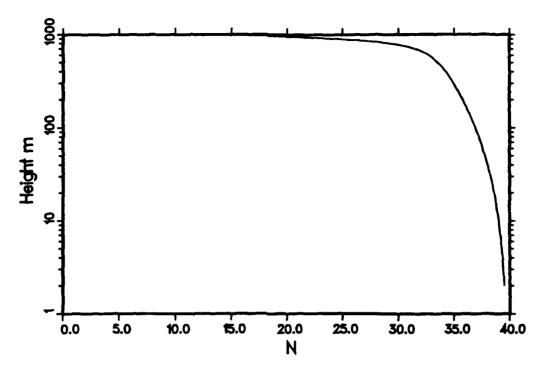


Figure 9. Wind turning angle, Nebraska data (8/19/53 16:35 CST) R/K optical profile fit with 4th degree polynomial fit for N. In N(z) = $-0.11031 + 3.08117 \times 10^{-3} z - 4.38265 \times 10^{-6} z^2 + 6.59899 \times 10^{-9} z^3 - 2.93911 \times 10^{-12} z^4$.

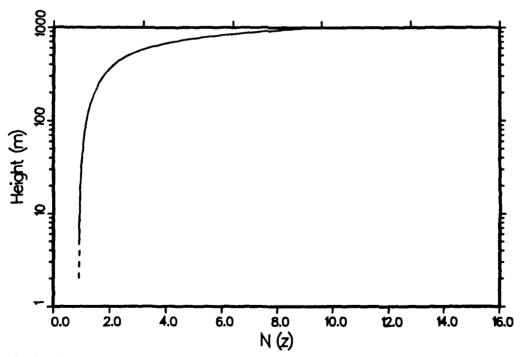


Figure 10. N(z) profile corresponding to figure 9.

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